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Simulation and Measurement of Angle Resolved Reflectance from Black Si Surfaces

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ABSTRACT: In this work angle-resolved reflectance from nanostructured Si surfaces realized by maskless RIE texturing has been simulated and measured. The simulation and experimental measurement data show the same trend. Experimentally a total reflectance below 1% for incident angles below 30° and specular reflectance below 0.1% at incident angles below 70° is seen. In both simulation and experiment the specular reflectance is below 10% at incident angles below 65° and below 1% at incident angles below 45° in the case of non-linear graded refractive index. From the simulation results the non-linear graded refractive index yields lower reflectance than the linearly graded refractive index.

Keywords: black silicon, reactive ion etching, angle dependence, reflectance, nanostructures

1 INTRODUCTION

Nanostructures etched in silicon surfaces such as reactive ion etch (RIE) textured black Si have shown to be potentially useful in photovoltaic applications [1-4]. In particular, the reduced reflectance over a broad range of incident angles [5] compared to that of bare silicon and silicon with a simple anti-reflection coating. Nguyen et al. [6] simulated the reflectance of nanostructures with peak heights of 900 nm as a function of incident angle. The investigation of angle-resolved optical behavior of nanostructured Si is particularly important considering the reported angle-dependence of power output [7-8] of commercial Si solar cells. This work differs from previous studies such as [6] by focusing on smaller nanostructures. The risk of increased surface recombination due to the etched nanostructures implies a compromise between optical performance and surface recombination. Thus, smaller nanostructures resulting in minimal surface recombination yet minimal reflectance are ideal. For this reason this work focuses on nanostructured surfaces with peak heights of 300 nm and two different graded refractive index schemes resembling experimentally fabricated surfaces relevant for photovoltaics.

In this work we have simulated and experimentally measured the reflectance from nanostructured silicon surfaces realized by mask-less RIE texturing. The reflectance was evaluated as a function of the incident angle of the light.

2 SIMULATION MODEL

To simplify modelling of the reflectance of the black silicon nanostructure a mean field approach was used; here the refractive index, n , was varied gradually - either linearly or non-linearly - from that of silicon, n_{Si} , to that of air, n_{air} , across a distance equal to the height, h , of the nanostructures according to

$$n(z) = \begin{cases} n_{Si} & , \text{ for } z \leq 0 \\ n_{air} & , \text{ for } z \geq h \\ n_{air}f(z, h, \Lambda) + n_{Si}[1 - f(z, h, \Lambda)] & , \text{ for } 0 < z < h \end{cases}$$

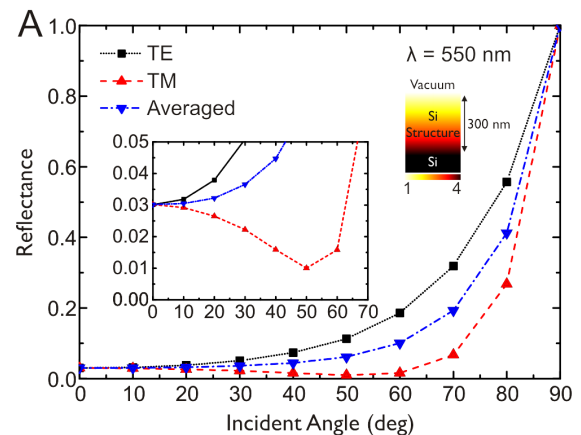
where Λ is a nonlinearity parameter. The index shape function was defined as $f(z, h, \Lambda) = \ln(1+z/\Lambda)/\ln(1+h/\Lambda)$ in case of a non-linear index profile and $f(z, h, \Lambda) = z/h$ in case of a linear index profile; here the parameters $\Lambda=10$ nm and $h=300$ nm were used. With this index profile the time-harmonic Maxwell equations were

solved in the form of the Helmholtz equations (e.g. $\nabla^2 \mathbf{E} = -k^2 \mathbf{E}$, where k is the wavenumber) for the electric and magnetic fields \mathbf{E} and \mathbf{H} , respectively. The calculation was done for the case of a plane optical wave of wavelength $\lambda=550$ nm incident at an angle θ to the surface normal. From the fields Poynting's vector $\mathbf{S} = \mathbf{E} \times \mathbf{H}$ and its time average z-components $\langle \mathbf{S} \rangle \cdot \mathbf{e}_z$ were calculated at the source and the detector, from which the reflectance R was calculated.

3 SIMULATION RESULTS

The results of the simulations are shown in the reflectance graphs in Fig.1 where reflectances for TE and TM waves are shown along with the mean reflectance of a 50/50 mixture of TE and TM waves as a function of the incident angle, the calculated reflectances in Fig. 1(a) are for a linearly graded index, while the reflectances for the nonlinear graded index are shown in Fig. 1(b). As expected, the reflectance is higher for TE than for TM waves. In all cases the reflectance is very low (less than 1% for non-linear graded index and less than 5% for linearly graded index) for incident angles below 45°.

At larger incident angles the reflectance increases rather steeply. We observe that the reflectance resulting from the non-linear graded index is generally lower than the linear graded index and stays below 1% until the incident angle is increased above 45°. In addition the difference in reflectance between TE and TM waves is less pronounced.



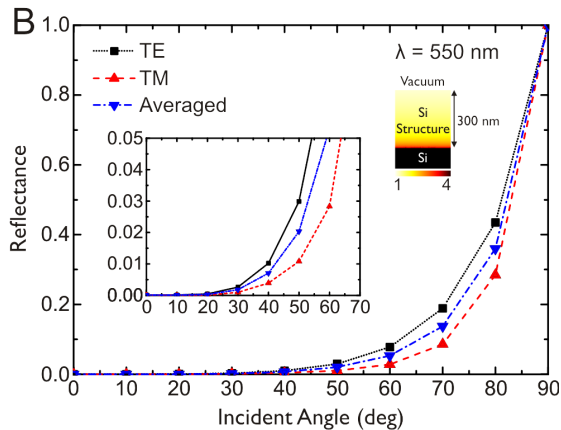


Figure 1: Simulated reflectance as function of incident angle at a wavelength of 550 nm for surfaces with nanostructures of 300 nm in height in case of (a) linearly graded refractive index, (b) non-linearly graded refractive index. The insets in (a) and (b) show the simulated reflectance at incident angles from 0-70°.

4 EXPERIMENTAL METHODS AND RESULTS

Black Si was realized by means of mask-less RIE at room temperature in O_2 and SF_6 plasma. The texturing process was carried out at a gas flow ratio of $O_2:Sf_6 \approx 1:1$, a pressure of 10-30 mTorr, a platen power of 30-100 W at 13.56 MHz in a STS RIE system. The resulting surface morphology was characterized using scanning electron microscopy (SEM), and SEM images of the structures are shown in Fig.2. The different morphologies shown in Fig.2 indicate that the graded refractive index profile may be approximately linear in some cases and non-linear to some extent in other cases.

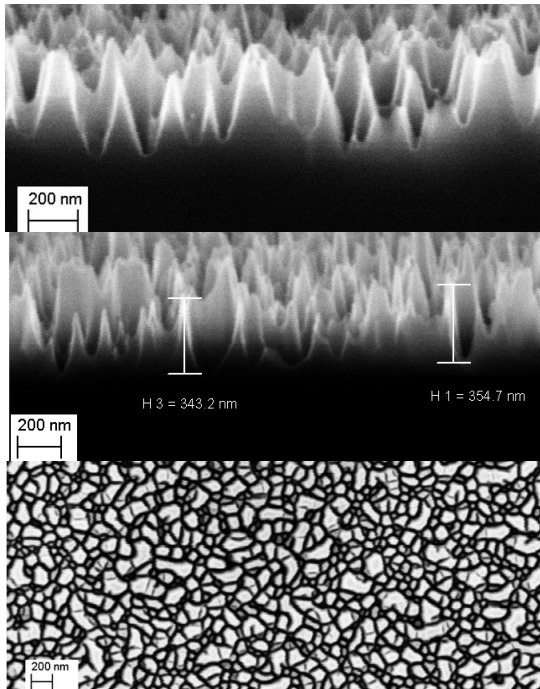


Figure 2: SEM-images at 45° (bottom) tilt of RIE-textured Si surfaces with 300 nm nanostructure height. The nanostructures represent approximately linear (top) and non-linear (middle) graded refractive index profiles.

The specular angular-dependent optical reflectance of the nanostructured silicon surface was measured for wavelengths in the range 300-1000 nm using a Woollam VASE ellipsometer.

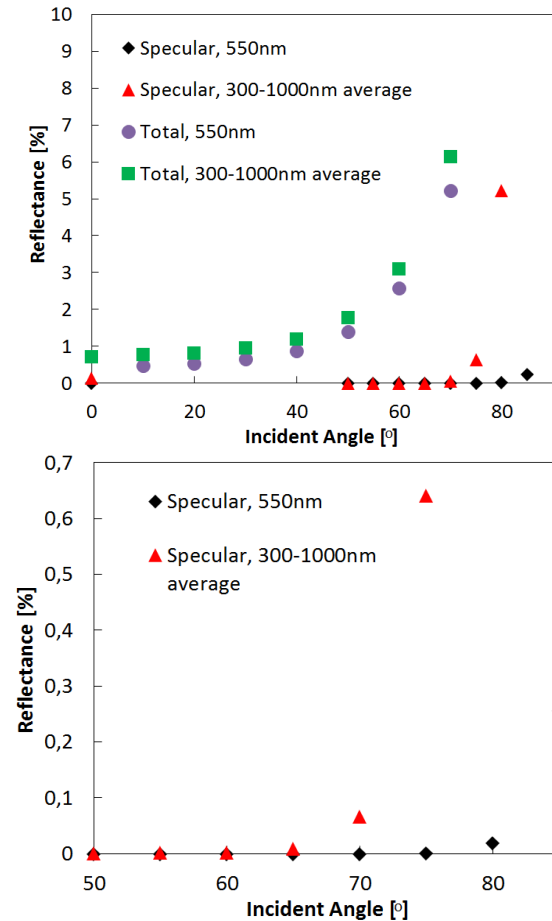


Figure 3: Experimental specular and total reflectance as a function of incident angle. The average reflectance in the wavelength range 300-1000 nm and the value at a wavelength of 550 nm (directly comparable to the simulation) are shown (top). The specular reflectance at incident angles of 50-85° is also shown (bottom).

Fig.3 shows the measured specular and total reflectance as a function of the incident angle. Both the average reflectance in the wavelength range 300-1000 nm and the reflectance at 550 nm are shown. The reflectance is seen to be dominated by non-specular reflection. In agreement with the simulation the specular reflectance is seen to be very low, but the experimental specular reflectance stays low even at very high incident angles (i.e. below 0.1% at angles below 65°). The measured total reflectance is more comparable in magnitude to and agrees quite well with the calculated reflectance. The reason is that due to the surface topology a major part of the reflected waves are reflected in a direction different from that of the detector in a specular reflection measurement set-up and escape detection.

We note that the simple simulation model - by construction - is unable to model real diffuse reflection; this can be accomplished using a much more detailed model of the nanostructured surface, which is part of future work.

7 CONCLUSION

Angle-resolved reflectance from nanostructured Si surfaces realized by mask-less RIE texturing has been simulated and measured. The simulation and experimental measurement data show the same trend. Experimentally a total reflectance below 1% for incident angles below 30° and specular reflectance below 0.1% at incident angles below 70° is seen. In both simulation and experiment the specular reflectance is below 10% at incident angles below 65° and below 1% at incident angles below 45° in the case of non-linear graded refractive index. From the simulation results the non-linear graded refractive index yields lower reflectance than the linearly graded refractive index. Modelling of the diffuse reflectance is part of future work.

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